About the influence of square-root Van Hove singularity on the critical temperature of high-Tc superconductors

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It is shown that the square-root Van Hove singularity in the density of states $\nu(E_F) \sim (E_F - E_0)^{-1/2}$, associated with the extended saddle-point features in the electronic spectra of cuprate metal-oxides with hole-type conductivity, leads to a nonmonotonic dependence of the critical temperature T_c on the position of the Fermi level E_F with respect to the bottom E_0 of the saddle. As the result of cancellation of the divergency of $\nu(E_F)$ in the electron-electron coupling constant, renormalized due to the account of strong coupling effects, T_c approaches zero in the limit $E_F \to E_0$, contrary to the case of the weak coupling approximation, which gives a finite (and close to maximal) value of T_c for $E_F \to E_0$. The dependence of T_c on the concentration of doped holes, obtained in the strong coupling approximation, agrees qualitatively with experimental data for the overdoped cuprate metal-oxides.

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1. The photo-emission spectroscopy experiments with high angular and energy resolution [1,2,3,4,5] show the existence of the extended saddle point features (ESPF) near the Fermi level in the electron spectra of the layered crystals of the cuprate metal oxides with hole-type conductivity ($YBaCuO$, $BiSrCaCuO$, $TlBaCaCuO$). These so called "flat" portions of spectra should give rise to a square-root Van Hove singularity in the electronic density of states $\nu(E_F) \sim (E_F - E_0)^{-1/2}$. The Fermi energy $\mu_1 \equiv (E_F - E_0)$ and the Fermi momentum $k_F \approx \sqrt{2m_1^*\mu_1}$ on these quasi one-dimensional portions with effective mass $m_1^* \gg m_0$ (where m_0 is the free electron mass) are anomalously small and for the optimally doped crystals equal $\mu_1 \simeq (20 \div 30)$ meV and $k_{F1} \simeq (0.15 \div 0.17)$ Å^{-1}, while the extension of the saddle anomalies in the momentum space is about $P_1 \simeq 0.5$ Å^{-1} [4,5].

As was shown in [2,6] in the framework of the BCS model [7], the ESPF with square-root Van Hove singularities lead, under the condition $\mu_1 \leq T_c$, to the nonexponential (power-like) T_c dependence on the dimensionless coupling constant of the effective interelectronic attraction λ: $T_c \approx \mu_1\lambda^2$, where $\lambda \approx \lambda_1\sqrt{E_1/\mu_1}$, i.e. the critical temperature approaches constant limit $T_c \approx E_1\lambda_1^2$ when $\mu_1 \to 0$. Thus, according to [2], for $E_1 \geq 1$ eV it is possible to obtain rather high values of $T_c \geq 100$ K even with small constant $\lambda_1 \sim 0.1$, regardless of the underlying mechanism for Cooper pairing of the current carriers.

Yet for large values of λ it is necessary to use the strong coupling approximation [8], which implies the renormalization of the coupling constant $\widetilde{\lambda} = \lambda/(1+\lambda)$ leading to the cancellation of the divergency $\lambda \sim \nu(\mu_1) \sim \mu_1^{-1/2}$ in the point $\mu_1 = 0$. As shown in the present paper, due to this cancellation $T_c \sim \mu_1$ when $\mu_1 \to 0$, that is T_c vanishes when the Fermi level touches the bottom of the extended saddle anomalies, contrary to the result of the weak coupling approach [2,6], when T_c has finite (and close to maximal) value at $\mu_1 = 0$. The nonmonotonic dependence of T_c on the concentration of doped holes n_p obtained with the account of the strong coupling effects qualitatively agrees with the experimental data for the overdoped cuprates [9,10].

2. We shall proceed from the assumption that the high-temperature superconductivity mechanism in the layered cuprate metal oxides is governed by the Cooper pairing of the fermions (electrons, holes) through the exchange of the virtual bosons (phonons, magnons, plasmons, excitons). In the strong coupling approximation the superconducting state is described by the set of equations for the normal Σ_1 and anomalous Σ_2 self-energy parts. Under the condition that the characteristic energy $\tilde{\Omega}$ of bosons, mediating in the interaction, is much greater then T_c, and with account for the quasi-2D character of the electron spectrum in the layered cuprates and the anisotropy of the electron-electron interaction, the linearized equation for the gap $\Delta(\mathbf{k},\omega)$ on the Fermi surface for $T \to T_c$ can be written as

$$(1+\lambda(\theta)) \cdot \Delta(\theta,0) = \frac{1}{2}\int_0^{2\pi}\frac{d\theta'}{2\pi}\int_{-\tilde{\Omega}}^{\tilde{\Omega}}\frac{d\omega}{\omega}\,\mathrm{Re}\,\Delta(\theta',\omega)\;\nu(\theta',\omega)\;W(\theta,\theta',\omega)\tanh\frac{\omega}{2T_c}, \tag{1}$$

where $\lambda(\theta) = -\partial\Sigma_1(\theta,\omega)/\partial\omega|_{\omega=0}$ is the dimensionless constant of the retarded interaction, $\Delta(\theta,\omega) =$

$\Sigma_2(\theta,\omega)/(1+\lambda(\theta))$ is the anisotropic gap in the quasiparticle spectrum, θ and θ' are the angles between one of the main crystallographic axes (**a** or **b**) in the plane of layers and the electron momenta $\mathbf{k}$ and $\mathbf{k}'$ lying on the Fermi surface, while $W(\theta,\theta',\omega)$ and $\nu(\theta,\omega)$ are the matrix element of the interelectron interaction and the electron density of states, respectively, which could be expanded into the Fourier series in the angles θ and θ'. For the sake of simplicity we shall use only the first terms in the expansion of $W(\theta,\theta',\omega)$, corresponding to the representations A_1 and B_1 of the symmetry group C_{4v} of the cuprate plane CuO_2:

$$W(\theta,\theta',\omega) = W_0(\omega) + W_2(\omega)\cos 2\theta\cos 2\theta' + W_4(\omega)\cos 4\theta\cos 4\theta', \tag{2}$$

and we shall write the anisotropic density of states in the vicinity of the closed and roughly cylindric Fermi surface (Fig. 1) as

$$\nu(\theta,\omega) = \nu_+(\omega) + \nu_-(\omega)\cos 4\theta; \qquad \nu_\pm(\omega) = \frac{1}{2}\left[\nu_1(\mu_1)\,\mathrm{Re}\sqrt{\frac{\mu_1}{\mu_{1+\omega}}} \pm \nu_2\right]. \tag{3}$$

Here $\nu_1(\mu_1) \sim \mu_1^{-1/2}$ is the density of states on the quasi-1D portions of the Fermi surface near the extended saddle points with square-root Van Hove singularity, and ν_2 is the constant density of states on the quasi-2D portions of the Fermi surface in the direction of the diagonals of the Brillouin zone. The anisotropic coupling constant $\lambda(\theta)$ is given in this case by

$$\lambda(\theta) = \lambda_0 + \lambda_4\cos 4\theta; \qquad \lambda_0 = \nu_+(\omega)\cdot W_0(0); \qquad \lambda_4 = \nu_-(\omega)\cdot W_4(0). \tag{4}$$

For sufficiently large positive values of $W_0(0)$ and $W_4(0)$ the s-wave symmetry of the Cooper pairing may prevail, resulting in superconducting state with the anisotropic gap

$$\Delta_s(\theta,\omega) = \Delta_0(\omega) + \Delta_4(\omega)\cos 4\theta. \tag{5}$$

The critical temperature T_c^s is given in this case by the solution of the fallowing set of the coupled integral equations (to simplify it we have neglected the frequency dependences of Δ and W in the frequency range $|\omega| < \tilde{\Omega}$):

$$(1+\lambda_0)\Delta_0 + \frac{1}{2}\lambda_4\Delta_4 = \frac{1}{2}W_0(0)\int_{-\tilde{\Omega}}^{\tilde{\Omega}}\frac{d\omega}{\omega}\left[\nu_+(\omega)\cdot\Delta_0 + \frac{1}{2}\nu_-(\omega)\cdot\Delta_4\right]\tanh\frac{\omega}{2T_c^s}; \tag{6}$$

$$(1+\lambda_0)\Delta_4 + \lambda_4\Delta_0 = -\frac{1}{4}W_4(0)\int_{-\tilde{\Omega}}^{\tilde{\Omega}}\frac{d\omega}{\omega}\left[\nu_+(\omega)\cdot\Delta_4 + \frac{1}{2}\nu_-(\omega)\cdot\Delta_0\right]\tanh\frac{\omega}{2T_c^s}. \tag{7}$$

On the other hand, for a high enough positive value of W_2 the $d_{x^2-y^2}$-wave symmetry of the Cooper pairing will dominate, with the resulting gap given by $\Delta_d(\theta) \sim \cos 2\theta$ and the critical temperature determined by the equation

$$1+\lambda_0 = \frac{1}{4}W_2(0)\int_{-\tilde{\Omega}}^{\tilde{\Omega}}\frac{d\omega}{\omega}\left[\nu_+(\omega) + \frac{1}{2}\nu_-(\omega)\right]\tanh\frac{\omega}{2T_c^d}. \tag{8}$$

3. As the majority of experiments (see i.e. [11,12,13,14]) indicate the $d_{x^2-y^2}$-wave gap symmetry in high-temperature superconductors, we shall consider only this case, corresponding in our model to the high value of W_2 in (2). Taking into account (3), the equation (8) for $\mu_1 < \tilde{\Omega}$ may be rewritten than as

$$1 = \frac{1}{4}\frac{W_2}{1+\lambda_0}\cdot\left[\frac{3}{2}\nu_1(\mu_1)\int_{-\mu_1}^{\tilde{\Omega}}\frac{d\omega}{\omega}\sqrt{\frac{\mu_1}{\omega+\mu_1}}\tanh\frac{\omega}{2T_c^d} + \nu_2\ln\left(\frac{\tilde{\Omega}}{T_c^d}\right)\right]. \tag{9}$$

The first term in square brackets in (9) corresponds to the quasi-1D portions of the Fermi surface with the square-root Van Hove singularity, while the second term describes the influence of the quasi-2D portions with the constant density of states.

The approximate integration over ω in (9) gives for $T_c^d \ll \mu_1$,

$$\left(T_c^d\right)^{3\alpha_1+\alpha_2} \approx \left(4\mu_1\right)^{3\alpha_1} \cdot \tilde{\Omega}^{\alpha_2} \cdot \exp\left\{-\frac{1+\lambda_0}{\lambda_2}\right\}, \tag{10}$$

where

$$\alpha_1 = \frac{\nu_1\left(\mu_1\right)}{\nu_1\left(\mu_1\right)+\nu_2}; \quad \alpha_2 = \frac{\nu_2}{\nu_1\left(\mu_1\right)+\nu_2}; \quad \lambda_2 = \frac{1}{2}\left(\nu_1\left(\mu_1\right)+\nu_2\right)\cdot W_2. \tag{11}$$

In the opposite case of $T_c^d \gg \mu_1$, when $\nu_1 \gg \nu_2$ and $\lambda_0 \approx \frac{1}{2}\nu_1 W_0$ at $\mu_1 \to 0$, the cancellation of ν_1 in the renormalized coupling constant reduces (9) to

$$T_c^d \approx 2\mu_1 \cdot \left(\frac{3W_2}{2W_0}\right)^2, \tag{12}$$

so that $T_c^d \to 0$ when $\mu_1 \to 0$. It is possible to show using (6) and (7) that in the strong coupling approximation the similar result ($T_c^d \sim \mu_1$ when $\mu_1 \to 0$) is valid for the s-wave gape symmetry as well, contrary to the result of [2,6], obtained in the weak coupling approximation, when T_c is finite at $\mu_1 = 0$ and close the maximal value.

The results of the numerical solution of eq. (8) are shown in Fig. 2. The T_c^d dependencies on μ_1 are represented for several values of parameters $\tilde{\Omega}$ and $\lambda_1 = \nu_1^* W_2$, where $\nu_1^* \equiv \nu_1\left(\mu_1^*\right)$ and $\mu_1^* \approx (0.02 \div 0.03)$ eV, which corresponds to the position of the Fermi level in the optimally doped cuprates [3,4]. Solid curves 1 and 2 are calculated for $\tilde{\Omega} = 0.1$ eV and $\tilde{\Omega} = 2$ eV respectively, with the fixed ratio $\nu_1^*/\nu_2 = 5$. The constants λ_1 and λ_0 where chosen so as to produce the position of the maximum of T_c^d in the point $\mu_1^* = 0.03$ eV and the maximal value of $T_c \approx 110$ K, experimentally observed in $BSCCO$ compounds. Notice that for the fixed ratio of the constants λ_1 and $\lambda_0\left(\mu_1^*\right)$ these constraints on the position and value of the T_c maximum lead to the power-law dependence of the constant λ_1 on $\tilde{\Omega}$ with a small exponent $\beta \approx -0.06$, shown with the log-log plot of the inset in Fig. 2. The value of the constant λ_1, necessary for achieving sufficiently high T_c, is relatively small and only weakly depends on the characteristic energy of the interaction, determined by the specific mechanism of the Cooper pairing. With the dashed curves in Fig. 2 are shown the dependencies of T_c^d calculated for the same parameters, but without the renormalization factor $(1+\lambda_0)$, which corresponds to the weak coupling approximation [2,6].

Fig. 3 represents the concentrational dependencies of T_c^d, corresponding to the curves 1 and $1'$ of Fig. 2, obtained with account for the expression for the density of states (3). The theoretical curves are compared to the experimental values, taken from [11], of the critical temperature for different hole concentrations n_p per Cu atom . We see the good agreement of the experimental data for the overdoped cuprates with the theoretical dependence $T_c\left(n_p\right)$, obtained in the strong coupling approximation.

In summary, we have shown that the effect of superconducting critical temperature decreasing with the increase in the hole concentration in the overdoped cuprates, with T_c eventually becoming zero at some concentration, is closely connected to the existence of the square-root Van Hove singularity in the electronic density of states. This conclusion is a consequence of the coupling constant renormalization due to the strong coupling effects, and does not depend on the specific mechanism of Cooper pairing and the symmetry of superconducting order parameter.

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Figure captions

Fig. 1 Cross section of the Fermi surface of the cuprate layered metal-oxides of the $BSCCO$ type. The closed hole-like Fermi surface is centered in the corner $(\pi/a, \pi/a)$ of the Brillouin zone.

Fig. 2 Critical temperature T_c in a function of the Fermi energy $\mu_1 = E_F - E_0$ on the extended saddle point features, calculated in the strong coupling (solid curves) and weak coupling (dashed curves) approximations. Curves 1 and $1'$ correspond to $\tilde{\Omega} = 0.1$ eV and $\lambda_1 = 0.68$, curves 2 and $2'$ – to $\tilde{\Omega} = 2$ eV and $\lambda_1 = 0.5$.

Fig. 3 Critical temperature T_c in a function of the hole concentration per Cu atom n_p. Theoretical curves correspond to curves 1 and $1'$ of Fig. 2. The experimental data are taken from [11]: • – $TlPbCaYSrCuO$ (1212) , △ – $BiPbSrLaCuO$ (2201)

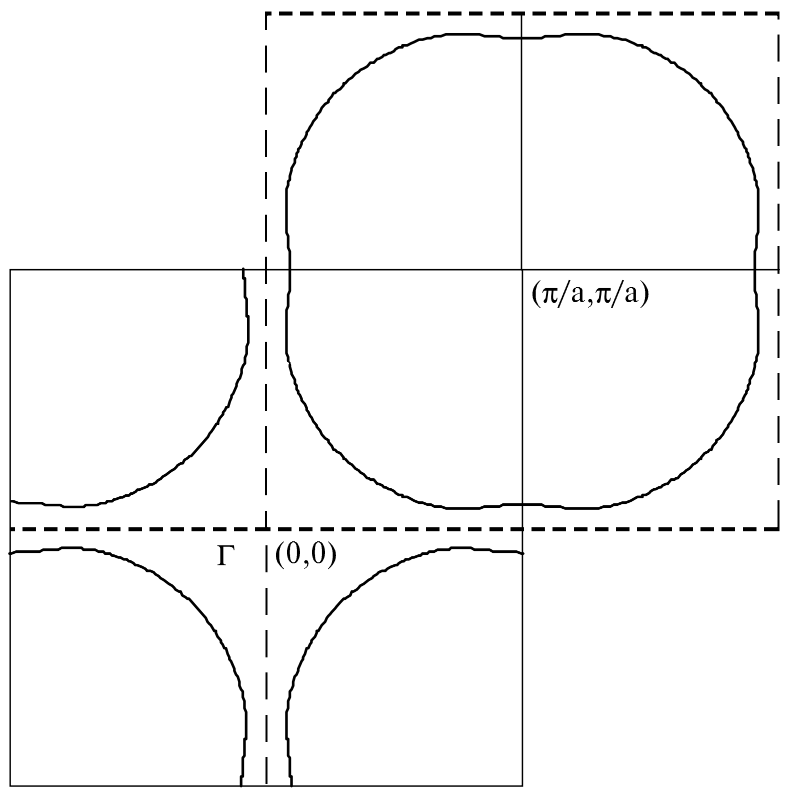
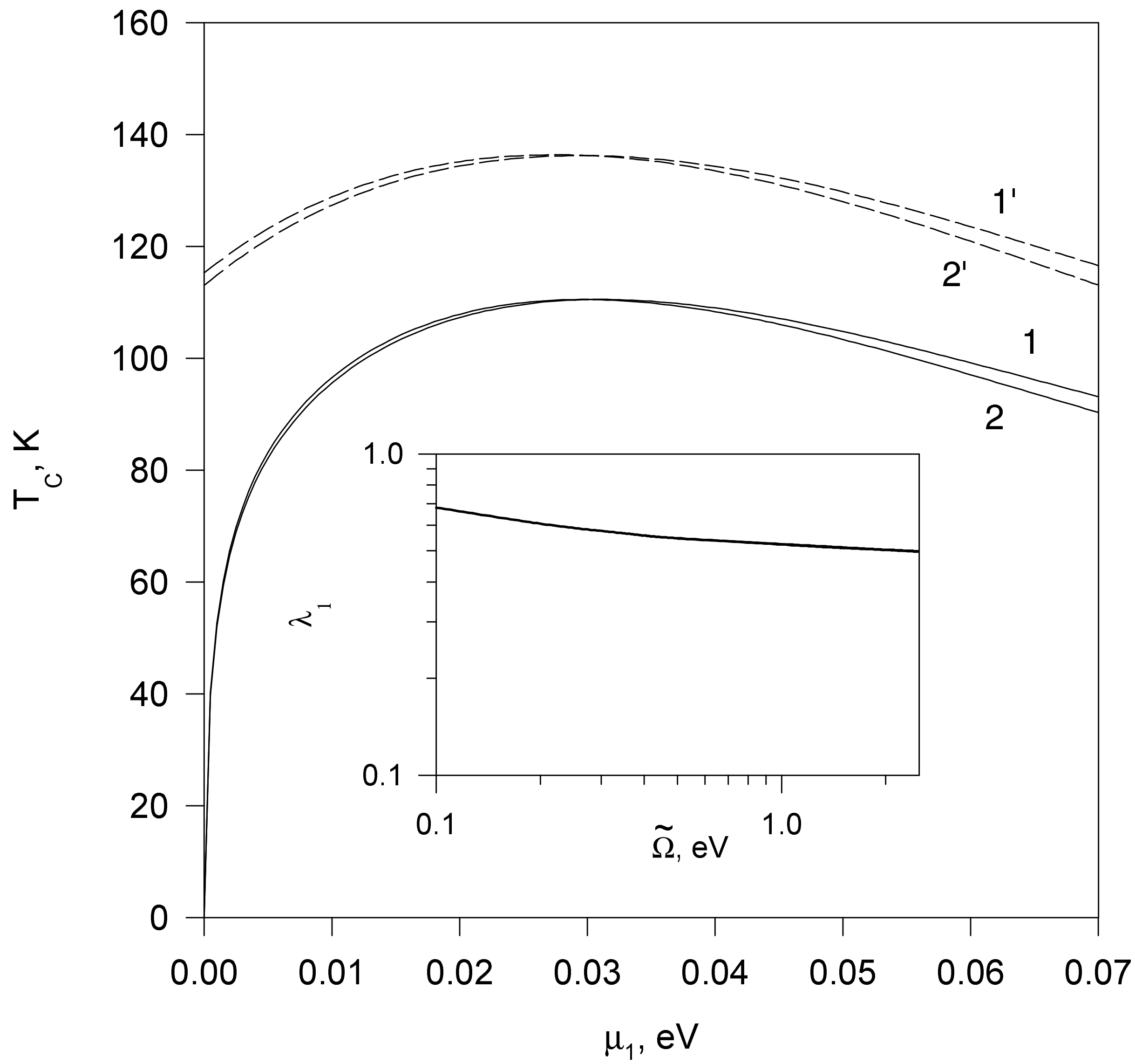


Fig. 1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140
120
100
80
60
40
20
0
T_c, K
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
μ_1, eV
1'
2'
1
2
1.0
0.1
λ_1
0.1
1.0
$\tilde{\Omega}$, eV

Fig. 2

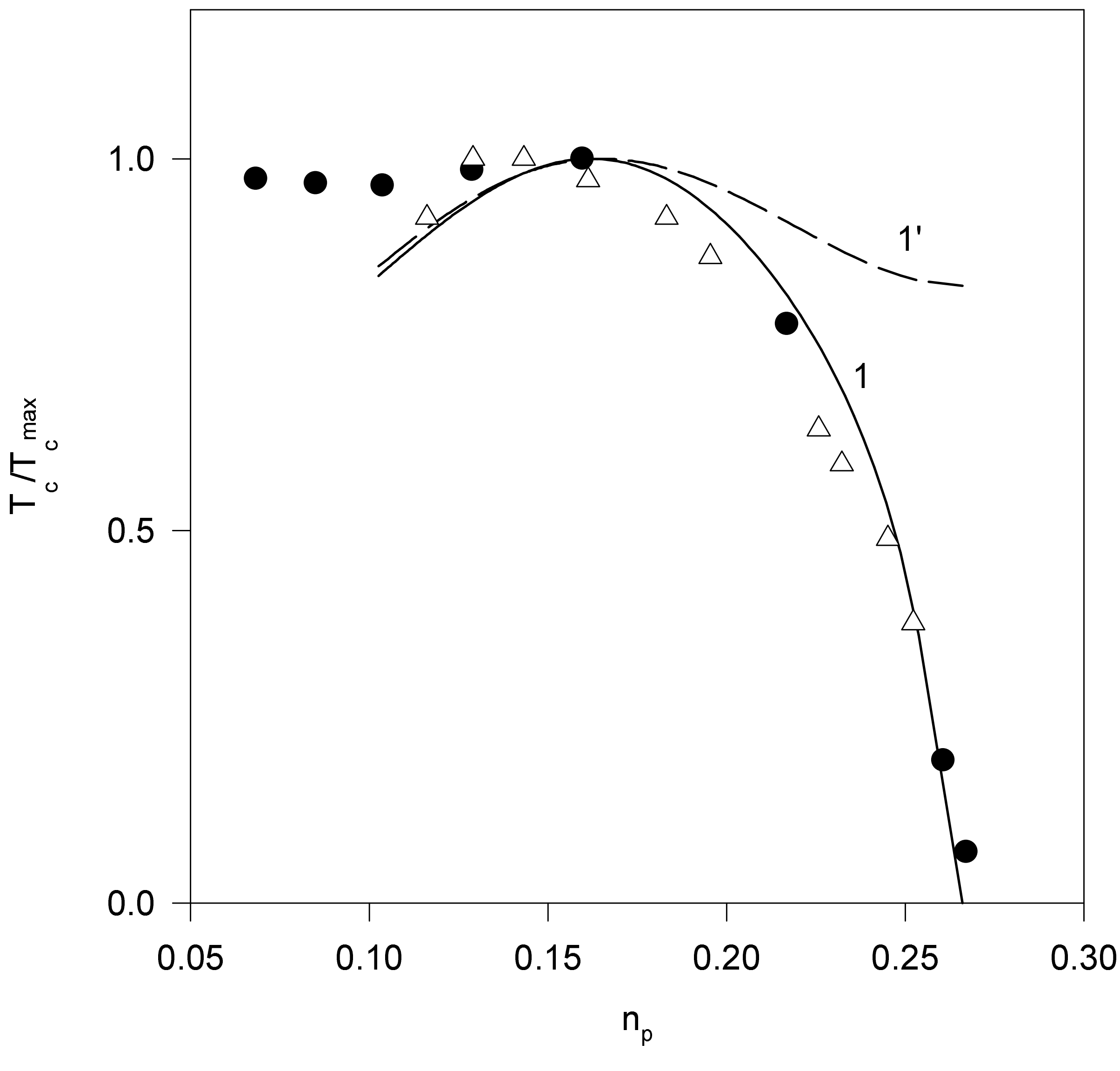

Fig. 3